# DFT insight into the polymerization mechanism of conjugated electroluminescent polymer PPV

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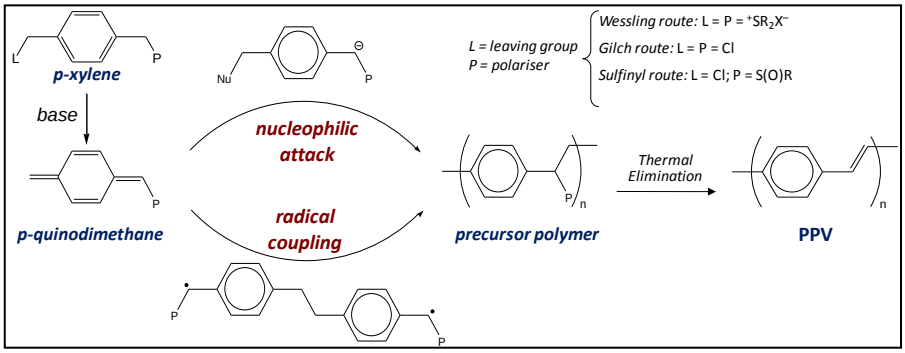
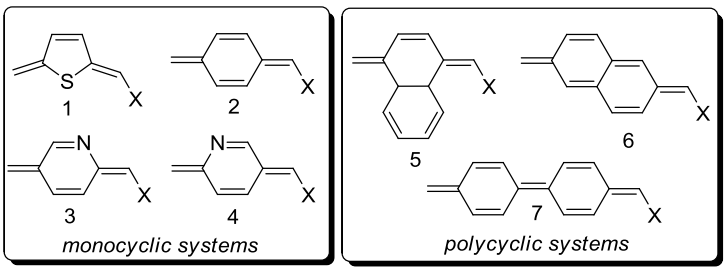
Despite various studies on the polymerization of PPV through different precursor routes, detailed mechanistic insight on the level of the individual reactions and intermediates is still incomplete. A recent study was performed to gain insight into the polymerization of PPV *via* the Gilch route –known to exclusively occur through a radical mechanism– and identify reactions that lead to side products, such as the p-cyclophane system.




Furthermore, the effect of the identity of the p-quinodimethane system on PPV polymerization was assessed with respect to the size of the aromatic core as well as heteroatoms in the conjugated system. The nature of the aromatic core and the specific substituents may alter the electronic structure of the p-quinodimethane monomers; hence affect the mechanism of polymerization. More specifically, it was suggested that the driving force for radical formation, is the re-aromatization of the p-quinodimethane systems.

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